Quantum Optical Random Walk: Quantization Rules and Quantum Simulation of Asymptotics

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Abstract

Rules for quantizing the walker+coin parts of a classical random walk are provided by treating them as interacting quantum systems. A quantum optical random walk (QORW), is introduced by means of a new rule that treats quantum or classical noise affecting the coin's state, as sources of quantization. The long term asymptotic statistics of QORW walker's position that shows enhanced diffusion rates as compared to classical case, is exactly solved. A quantum optical cavity implementation of the walk provides the framework for quantum simulation of its asymptotic statistics. The simulation utilizes interacting two-level atoms and/or laser randomly pulsating fields with fluctuating parameters.

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I. INTRODUCTION

Discrete quantum random walks on a line, [2],[3],[8],[9], (for a review in a more general setting see [1]) is a paradigmatic construction of a quantum system performing a motion similar to the usual classical discrete random walk on a line, but with a number of important differences like the quantum treatment of its coin and walker systems, the role of quantum entanglement, novel diffusion and hitting properties of its motion etc. The asymptotic behavior of such walks has been studied in [9],[10],[21]. Also important theoretical suggestions about the utilization of those properties in the construction of quantum algorithms that would outperform classical rivals in tasks such as searching a database etc, have been put forward, see e.g. [4]. The effect of decoherence on the evolution of discrete quantum walks has been studied in e.g. [15],[16]. Experimental proposals also exists concerning e.g. quantum coin-tossing, and quantum diffusion see e.g. [11],[26],[14],[12], [13]. The coin control over discrete quantum walks on graphs has been studied in [20]. Continuous time quantum walks on graphs, which are defined without the use of a coin, were studied in e.g. [6],[7], and their potential implementation for the construction of fast search algorithms were studied in [5].

The present work extends previous ones on the so called V^k models of quantum discrete walks on a line[22][23][24][25]. Its aim is twofold: first to argue that a general and systematic framework of quantization of classical walks is possible and well physically motivated, and second to study the walk beyond transient dynamics in its asymptotic regime and to show the possibility of simulating its statistical behavior in terms of another quantum system, introducing thus the quantum simulation of a quantum walk. This double aim is achieved by introducing the Quantum Optical Random Walk (QORW); a mathematical model that refers to a typical cavity QED type of arrangement where a beam of two-level atoms passes through an optical cavity. [Technical caveat: although the mathematical description of cavity field done here is not the usual one i.e. in terms of the boson degree of freedom, but instead is in terms of states with positive and negative valued energy also (canonical algebra vs. Euclidean algebra, see below), appropriate truncations can be introduced in order to have only positive energy states (c.f. e.g. [12]); this remedy for the problem however will not be discussed here.]

The outline of the paper goes as follows: in Chapter II, the study of quantization rules is

developed, the QORW is introduce in Chapter III and several example of walks are solved; Chapter IV treats the walk in its asymptotic regime and introduces the technique of quantum simulation, examples of numerically simulated asymptotic probability density functions are provided; conclusions are summarized in last Chapter V.

II. QUANTIZATION RULES FOR CLASSICAL RANDOM WALKS

The essential feature of a simple QRW on a line is the promotion of mathematical correspondence: *left/right*$\rightarrow$ *head/tails,* between *walker*'s move directions and *coin*'s two sides, to a dynamical interaction among two physical systems. This is realized by introducing state Hilbert spaces $H_w = span(|m\rangle)_{m\in Z}$ and $H_c = span(|+\rangle, |-\rangle)$, for quantum walker and coin systems respectively. In H_w operates the Euclidean algebra with generators the *step operators* $E_\pm|m\rangle = |m \pm 1\rangle$,(and their their powers e.g. for $a > 0$, $(E_\pm)^a|m\rangle \equiv E_{\pm a}|m\rangle = |m \pm a\rangle$), and the *position operator* $L|m\rangle = m|m\rangle$. They satisfy the commutation relations $[L, E_\pm] = \pm E_\pm$, $[E_+, E_-] = 0$. Also important is the Fourier basis $H_w = span(|\phi\rangle = \frac{1}{2\pi}\sum_{m\in Z} e^{im\phi}|m\rangle, 0 \leq \phi < 2\pi)$, which is the eigenbasis of step operators viz. $E_\pm|\phi\rangle = e^{i\phi}|\phi\rangle$. In the coin space the projection operators $P_\pm = |\pm\rangle\langle\pm|$, are needed in order to realize the coin-tossing that drives the walk. Indeed one step of classical random walk (CRW), is described by means of the unitary $V_{cl} = P_+ \otimes E_+ + P_- \otimes E_-$. Its conditional action on walker states realizes the coin-tossing and the subsequent move of walker.

Explicitly the coin ρ_c and walker ρ_w, density matrices initially taken in product form $\rho_c \otimes \rho_w$, are assumed to interact unitarily by the transformation $\rho_c \otimes \rho_w \rightarrow V_{cl}(\rho_c \otimes \rho_w)V_{cl}$.Subsequently the two systems are decoupled by an unconditional measurement of the coin subsystem realized by means of the partial trace i.e. $V_{cl}(\rho_c \otimes \rho_w)V_{cl} \rightarrow Tr_c(V_{cl}(\rho_c \otimes \rho_w)V_{cl})$; the latter constitues the dynamical realization of the coin tossing process. The resulting walker density matrix $\varepsilon_{V_{cl}}(\rho_w) = Tr_c(V_{cl}(\rho_c \otimes \rho_w)V_{cl})$,written in the eigenbasis states of position operator L (see above), provides by means of its diagonal elements the occupation probability distribution $p_m = \langle m|\varepsilon_{V_{cl}}(\rho_w)|m\rangle$, of the states of walker system. This distribution in the course of time steps of the walk $n = 1, 2, ...,$ is identified with the occupation probabilities of the classical random walk on integers i.e. $p_m^{(n)} = \langle m|\varepsilon_{V_{cl}}(\rho_w^{(n)})|m\rangle, m = 0, \pm1, \pm2, ...,$with bias determined by the elements of ρ_c. Due to this the $\varepsilon_{V_{cl}}$ map is conceived as realization of CRW, which we next seek to quantize.

Quantization of CRW is conceived as the incorporation in coin space of an additional unitary operator U, the coin reshuffling matrix, so that the one-step operator now becomes $V = V_{cl}U \otimes \mathbf{1}$. To facilitate conceptual comparisons this procedure was christened $U-$quantization in ref. [25]. Almost all work that has been done in the area of quantum random walks, has been based on the scheme of $U-$quantization or modifications thereof. One particular class of such $U-$quantized walks are the V^k-models for which the one-step evolution of the walker's density matrix is given by the CPTP map ε_{V^k} as $\varepsilon_{V^k}(\rho_w) = Tr_c V^k(\rho_c \otimes \rho_w)V^{\dagger k}$[27].

Next we introduce a generalized version of the previous quantization method, the $\varepsilon-$quantization rule, which employs a positive and completely positive trace preserving map ε, acting on the coin density matrices, which is not necessarily taken to be unital, namely $\varepsilon(\frac{1}{2}\mathbf{1}) \neq \frac{1}{2}\mathbf{1}$. Then the one-step evolution of walker's density matrix of an $\varepsilon-$quantized model of a classical walk is defined as

$$\varepsilon_V(\rho_w) = Tr_c V_{cl}\varepsilon \otimes \mathbf{1}(\rho_c \otimes \rho_w)V_{cl}^{\dagger}. \tag{1}$$

In general for a V^k quantum walk model we will have that

$$\varepsilon_{V^k}(\rho_w) = Tr_c \left[V_{cl}\varepsilon_k \otimes \mathbf{1} ... \left(V_{cl}\varepsilon_1 \otimes \mathbf{1}(\rho_c \otimes \rho_w)V_{cl}^{\dagger}\right) ... V_{cl}^{\dagger}\right], \tag{2}$$

where in general a different quantizing CP map ε can be used between coin+walker interactions. To appreciate the changes brought about by $\varepsilon-$quantization we use the adjoint action of e.g operator X, on a density matrix defined as $AdX(\rho) = X\rho X^{\dagger}$,with property $AdXY(\rho) = AdXAdY(\rho)$. We assume that the ε map is determined by a set of Kraus operators as $\varepsilon(\rho_c) = \sum_i S_i\rho_c S_i^{\dagger}$, or in terms of the adjoint action $\varepsilon(\rho_c) = \sum_i AdS_i(\rho_c)$,[28]. To contrast deference between the usual $U-$quantization and the proposed $\varepsilon-$quantization rules we write the evolution map of the former as

$$\begin{aligned} \varepsilon_{V^k}(\rho_w) &= Tr_c \left(AdV_{cl}AdU\right)^k (\rho_c \otimes \rho_w) \\ &= Tr_c \left(Ad(V_{cl}U)\right)^k (\rho_c \otimes \rho_w), \end{aligned} \tag{3}$$

and the evolution map of the latter as

$$\begin{aligned} \varepsilon_{V^k}(\rho_w) &= Tr_c \left(\sum_i AdV_{cl}AdS_i\right)^k (\rho_c \otimes \rho_w) \\ &= Tr_c \left(\sum_i Ad(V_{cl}S_i)\right)^k (\rho_c \otimes \rho_w). \end{aligned} \tag{4}$$

It is evident from above that the $\varepsilon-$quantization rule applies a sum of adjoints at each factor of the $k-$fold product. This sum in addition to V_{cl}, is determined by the Kraus generators of the quantization map ε. In the simplest case where there is only one single unitary Kraus generator, the $\varepsilon-$ rule reduces to the $U-$quantization rule. The inclusion of Kraus generators in the quantization of classical walk, may stem from the fact of a hidden quantum interaction between the coin system and another unobserved quantum system, or it may be due to some classically fluctuating parametric variance of the coin system, that is treated on the average; generically we may say that it is due to quantum or classical noise. (see also previous studies of non-unitary models [11, 12, 14, 17, 18, 19], The number of Kraus generators as well as their matrix type provide in any case a flexible framework in which the quantization map may incorporate complex physical processes in coin systems that may take place within a evolution step of the walk.

III. QUANTUM OPTICAL RANDOM WALK

As an application of the $\varepsilon-$quantization rule we introduce a new kind of quantum walk. To this end we need to introduce a continuous family CPTP maps $\mathbf{E} = \{t \to \varepsilon_t, t \geq 0\}$, acting on the space of coin density matrices, where variable t is taken to stand for time. Among members of family $\mathbf{E}$, there exists a semi-group composition law, i.e $\varepsilon_{t_1} \circ \varepsilon_{t_2} = \varepsilon_{t_1+t_2}$.Also the identity map $\varepsilon_0 = id$, is included in $\mathbf{E}$.

Now we come to the Quantum Optical Random Walk; it physically outlines the crossing of an beam of two-level atoms, the *coins,* through a quantum optical cavity which sustains a standing quantum mode identified with the *walker* system. The walker+coin interaction realizes a V^2 QRW model, and it also takes into account the interaction of coin with some external environment, formalized as some CPTP time dependent map ε_t. This external interaction of the coin is taken to have been initiated at some past time 0, and to continuously happen in time while atom crosses the cavity. Entering into the cavity at some time t, in state $\varepsilon_t(\rho_c)$, the atom interacts instantaneously, being the coin part of QRW, with the walker/cavity mode. For the V^2 model two such coin+walker interactions occur: one interaction at time t, that changes their combine state as $\varepsilon_t(\rho_c) \otimes \rho_w \to V_{cl}(\varepsilon_t(\rho_c) \otimes \rho_w)V_{cl}^\dagger$, and a second one later on at time $t + \tau$, that effects the change of state: $V_{cl}(\varepsilon_t(\rho_c) \otimes \rho_w)V_{cl}^\dagger$ $\to V_{cl}(\varepsilon_\tau \otimes \mathbf{1}(V_{cl}(\varepsilon_t(\rho_c) \otimes \rho_w)V_{cl}^\dagger))V_{cl}^\dagger$. The V_{cl} 's are realized by sudden on-off switches of

the mode+atom interaction, possibly by driving the cavity mode off resonance. Then the two interactions taken together constitute one step of the walk. Subsequently the atom is considered leaving the cavity, the time clock is been reset, and a new atom is entering the cavity.(A realistic cavity QED model for implementing QRW in atom+mode interactions has been proposed in [12].) Explicitly the total change of walker's density matrix between two successive steps is given by the equation

$$\rho_w^{(n)} = \varepsilon_{V^2}(\rho_w^{(n-1)}) = Tr_c\left[AdV_{cl}\cdot\varepsilon_\tau\otimes\mathbf{1}\cdot AdV_{cl}\cdot\varepsilon_t\otimes\mathbf{1}\cdot(\rho_c\otimes\rho_w^{(n-1)})\right], \tag{5}$$

for $n = 1, 2, ...$,or more explicitly

$$\rho_w^{(n)} = \varepsilon_{V^2}(\rho_w^{(n-1)}) = \sum_{ijk=\pm1}\langle i|\varepsilon_t(\rho_c)|j\rangle\langle k|\varepsilon_\tau(|i\rangle\langle j|)|k\rangle E_{i+k}\rho_w^{(n-1)}E_{j+k}. \tag{6}$$

This shows that the $\varepsilon-$quantized V^2 walk proceeds with steps of length 0 and 2,on the ladder of walker states, with weights determined by the time dependent CPTP ε_t.This same map actually serves as the source of quantization of classical V_{cl}^2 walk. It is important however to emphasize that in this walk the physical origin of quantization is not an ad hoc imposed unitary rotation matrix in coin space, as it has been in most cases following the $U-$quantization rule, but instead it is the physical process of natural interaction of coin system with some external agent. As an example we can consider the case of a Rabi oscillating two-level atom that decays spontaneously. Such physical conditions render the $\varepsilon-$generalization of quantization for a classical walk a well motivated one.

The one-step map ε_{V^2} previously introduced is determined by parameters; these are some e.g λ parameter measuring the strength of ε_t, and the parameters t and τ, determining the time intervals of coin+walker interactions. Those time parameters should be finely tuned, so that is possible for the two interactions to take place during the time the atom/coin spends in the cavity. This can be decided by selecting the velocity of the atomic beam crossing the cavity.

To proceed with the problem of time evolution we introduce walker's density matrix, $\rho_w = \int_0^{2\pi}\int_0^{2\pi}\rho(\phi,\phi')|\phi\rangle\langle\phi'|d\phi d\phi'$. Due to linearity of evolution we only need to compute

$$\begin{aligned}\varepsilon_{V^2}(|\phi\rangle\langle\phi'|) &= Tr_c\left(V_{cl}(\phi)\varepsilon_\tau\left(V_{cl}(\phi)\varepsilon_t(\rho_c)V_{cl}(\phi')^\dagger\right)V_{cl}(\phi')^\dagger\right)|\phi\rangle\langle\phi'| \\ &\equiv A(\phi,\phi')|\phi\rangle\langle\phi'|,\end{aligned} \tag{7}$$

then

$$\varepsilon_{V^2}^n(\rho_w) = \int_0^{2\pi}\int_0^{2\pi}\rho(\phi,\phi')A(\phi,\phi')^n|\phi\rangle\langle\phi'|d\phi d\phi'. \tag{8}$$

In formulas above matrix $V_{cl}(\phi)$, is defined in the eigenbasis of step operators as $V_{cl} = \int V_{cl}(\phi)|\phi\rangle\langle\phi|d\phi$,where $V_{cl}(\phi) =$diag$(e^{i\phi}, e^{-i\phi})$. Namely in ϕ-basis we have that $E_{\pm} = e^{\pm i\Phi}$, where $\Phi = \int \phi|\phi\rangle\langle\phi|d\phi$, is a Hermitean phase angle operator.

The discrete distribution determining the m-th site occupation probability on the walker's ladder after n steps is

$$P_m^{(n)} \equiv \langle m|\varepsilon_{V^2}^n(\rho_w)|m\rangle = \frac{1}{(2\pi)^2}\int_0^{2\pi}\int_0^{2\pi} d\phi d\phi' A^n(\phi,\phi')e^{-im(\phi-\phi')}. \tag{9}$$

Change to variables $\phi_{\pm} = \phi \pm \phi'$, in the preceding expression shows that *if* $A(\phi_+, \phi_-)$, *is independent from variable* ϕ_+, then the ϕ_+ integral can be carried out and the probability becomes

$$P_m^{(n)} \equiv \langle m|\varepsilon_{V^2}^n(\rho_w)|m\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\phi_-\ A^n(\phi_-)e^{-im\phi_-}, \tag{10}$$

then the $A(\phi_-)$ can be identified with the characteristic function of the transition probability function of a classical random walk[33]. This is a general result independent of quantization rule that can be used as a *criterion of classicality* of quantum walk. Let us give some examples of classical walks quantized according to U and ε rules, and impose on them the criterion of classicality.

Examples from $U-$quantization rule:

i) The V model with evolution $\varepsilon_V(\rho_w^{(n)}) = Tr_c V\rho_c \otimes \rho_w^{(n-1)}V^{\dagger}$, gives $A_V(\phi_+,\phi_-) = \langle +|\rho_c|+\rangle e^{i\phi_-} + \langle -|\rho_c|-\rangle e^{-i\phi_-}$.This fulfills the classicality criterion and essentially leads to classical occupation probabilities drawn from the diagonal elements of walker's density matrix.

ii) The V^2 model with evolution $\varepsilon_V(\rho_w^{(n)}) = Tr_c V^2\rho_c \otimes \rho_w^{(n-1)}V^{2\dagger}$, initial $\rho_c = |+\rangle\langle +|$, and reshuffling matrix $U_{\frac{\pi}{4}} = e^{i\frac{\pi}{4}\sigma_2}$, been a $\frac{\pi}{4}$-rotation. This gives [24]

$$A_{V^2}(\phi_+,\phi_-) = \cos^2\phi_- - i\cos\phi_+\sin\phi_-. \tag{11}$$

The asymptotic characteristic function (cf. eq.(22)), that determines the limiting probabilities of the walk, is for this example

$$h(\phi) = -i\left[\partial_\phi A(\phi,\phi')\right]_{\phi'=\phi} = -\cos 2\phi. \tag{12}$$

Examples from $\varepsilon-$quantization rule:

iii) Assume initially we have a coin being in some mixed state ρ_c =diag$(q, 1-q)$, $0 \leq q \leq 1$, and that it suffers spontaneous de-excitation of its upper state with rate λ, then its state is described by the map [28],

$$\varepsilon_t(\rho_c) = S_0(t)\rho_c S_0^\dagger(t) + S_1(t)\rho_c S_1^\dagger(t), \tag{13}$$

where $\cos(\lambda t) = \sqrt{1-e^{-2\lambda t}}$, and

$$S_0(t) = \begin{pmatrix} \cos(\lambda t) & 0 \\ 0 & 1 \end{pmatrix}, \; S_1(t) = \begin{pmatrix} 0 & 0 \\ \sin(\lambda t) & 0 \end{pmatrix}. \tag{14}$$

Such a coin enters the cavity in state $\varepsilon_t(\rho_c)$ =diag$(q\cos^2\lambda t, -q\cos^2\lambda t + 1)$. Then we obtain that

$$A_{V^2}(\phi_+, \phi_-) = e^{-i2\phi_-}(1 - q\cos^2\lambda t) + e^{i2\phi_-} q\cos^2\lambda t \cos^2\lambda\tau + q\cos^2\lambda t \sin^2\lambda\tau \tag{15}$$

For $q = \frac{1}{2}$, we have the initial density matrix $\rho_c = \frac{1}{2}\mathbf{1}$, as special case. The criterion of classicality is also fulfilled here, so the diagonal elements of evolved walker's density matrix can be identified with a classical distribution.

Statement : Direct calculation verifies the general statement that classicality prevails in any $\varepsilon-$quantized V^k model, independently from the initial condition of coin system, as long as the quantization proceeds by employing an ε quantization map with Kraus generators being matrices having only diagonal or only anti-diagonal elements; such examples of ε maps are e.g the X, Y, Z, the depolarization channels, the mentioned spontaneous emission channel, as well as the transformation induced on the coin/atom after tracing out the bosonic field freedom in Jaynes-Cummings model and in its various modifications (c.f. [24, 25]).

iv) If initially we have a coin being in some mixed state ρ_c =diag$(q, 1-q)$, $0 \leq q \leq 1$, but $q \neq \frac{1}{2}$, and if the quantization proceeds by using the map

$$\varepsilon(\rho_c) = R_0\rho_c R_0^\dagger + R_1\rho_c R_1^\dagger, \tag{16}$$

where

$$R_0 = \frac{1}{\sqrt{2}}\mathbf{1}, \; R_1 = \frac{1}{\sqrt{2}}U_{\frac{\pi}{4}}, \tag{17}$$

we then obtain that

$$A_{V^2}(\phi_+, \phi_-) = \frac{3(1+2q)}{16}e^{i2\phi_-} + \frac{3(1-2q)}{16}e^{-i2\phi_-} + \frac{i(1-2q)}{4}\sin\phi_-\cos\phi_+ + \frac{1}{4}. \tag{18}$$

For $q = 0, 1$, we have the initial density matrix $\rho_c = |-\rangle\langle -|, |+\rangle\langle +|$, respectively. By comparing examples *ii*) and *iv*) we see that we pass from the $U-$quantization rule of the former to the $\varepsilon-$ quantization rule of the latter by simply mixing the reshuffling unitary matrix $U_{\frac{\pi}{4}}$ with the unit matrix. Such mixing is relevant in cases where there is probabilistic uncertainty as to whether reshuffling matrix is applied or not.

The criterion of classicality is not satisfied here, therefore we have a genuine ε-quantized random walk. By virtue of eq.(18), the asymptotic characteristic function is (c.f. eq.(22))

$$h(\phi) = -\frac{3}{4} + \frac{1-2q}{4}\cos 2\phi. \tag{19}$$

Closing this section we note that both quantization rules give non trivial models for quantum walks and that in some cases, as e.g in the last example the $\varepsilon-$rule is presented as a necessary amendment of U-rule when the latter can not be applied since the reshuffling matrix is either not exactly known or is not accurately applied.

IV. QUANTUM SIMULATION OF ASYMPTOTICS

Asymptotics: The dynamics of quantum walk can be described by the quantum statistical moments of the observable of *position operator* L, evaluated e.g after n steps. We obtain for its statistical moments

$$\langle L^s\rangle_n \equiv Tr(L^s\rho_w^{(n)}) = \frac{1}{2\pi i^s}\int_0^{2\pi} d\phi \left[\partial_\phi^s \left[\rho(\phi,\phi')A^n(\phi,\phi')\right]\right]_{\phi'=\phi}. \tag{20}$$

Next we study the asymptotic behavior of moments when the number of steps n is large. In this case we have that

$$\begin{aligned}\langle L^s\rangle_n &= \frac{n^s}{2\pi i^s}\int_0^{2\pi} d\phi\rho(\phi,\phi)\left[\partial_\phi A(\phi,\phi')\right]^s_{|\phi'=\phi} + O(n^{s-1}) \\ &\equiv \frac{n^s}{2\pi}\int_0^{2\pi} d\phi\rho(\phi,\phi)h(\phi)^s + O(n^{s-1}).\end{aligned} \tag{21}$$

Here we have introduced the *asymptotic characteristic function* (acf) $h(\phi)$, of the walk as

$$h(\phi) = -i\left[\partial_\phi A(\phi,\phi')\right]_{\phi'=\phi}. \tag{22}$$

The scaled by time limiting statistical moment of position operator is then obtained to be

$$\left\langle \left(\frac{L}{n}\right)^s \right\rangle_\infty \equiv \frac{1}{2\pi}\int_0^{2\pi} d\phi \rho(\phi,\phi) h(\phi)^s. \tag{23}$$

For the U-quantized ε_{V^k} model since $h(\phi) = \mathrm{Im}Tr_c(V^{k\dagger}(\phi)V^k(\phi)\rho_c)$, as can be obtained by elaborating on last equation, we have that

$$h(\phi) = Tr_c\left[(\sigma + V^\dagger(\phi)\sigma V(\phi) + \cdots + V^{\dagger k-1}(\phi)\sigma V^{k-1}(\phi))\rho_c\right], \tag{24}$$

where $\sigma = U^\dagger \sigma_3 U$ is a rotated σ_3 Pauli matrix.

It is important to note that the limiting positional moments provide all necessary information for a sufficient understanding of the ensuing walker asymptotic dynamics, and as seen from above these moments are expressed as classical mean values of the powers of function $h(\phi)$ of the stochastic variable ϕ, that takes values around a circle with pdf $\frac{1}{2\pi}\rho(\phi,\phi)$. Hence we will seek the exact knowledge of function $h(\phi)$ next, by the technique of quantum simulating the system of walk.

Quantum Simulation: The concept of quantum simulation of dynamics or statistics of a quantum system by another quantum system constitute a final goal for Quantum Information Science, since an alleged universal quantum computer device would function as an efficient simulator of any quantum process. In more modest claims a special purpose quantum system could be constructed and set up to interact with its environment, so that its dynamical or statistical behavior would simulate the respective dynamics or statistics of a given quantum system. The simulator system is possibly different from the original system, in e.g its dimension, type of interactions or necessary physical and computational resources required from its time evolution. However both original and simulator systems are both governed by laws of quantum mechanics[29, 30, 31, 32].

To construct a quantum simulation of asymptotic behavior of U-quantized walk, we proceed by simulating quantum mechanically its asymptotic characteristic function $h(\phi)$. Let us refer to eq.(24), and introduce firstly the CPTP map

$$\varepsilon^*_\phi(\sigma) = \frac{1}{k}(\sigma + V^\dagger(\phi)\sigma V(\phi) + \cdots + V^{\dagger k-1}(\phi)\sigma V^{k-1}(\phi)), \tag{25}$$

then we cast acf of eq.(24), in the form $h(\phi) = kTr_c(\varepsilon^*_\phi(\sigma)\rho_c)$. Equivalently we can express acf in the form $h(\phi) = kTr_c(\varepsilon_\phi(\rho_c)\sigma)$, where utilizing the cyclic property of trace, the dual

map ε_ϕ of the preceding map ε^*_ϕ, has been used that reads

$$\varepsilon_\phi(\rho_c) = \frac{1}{k}\left(\rho_c + V(\phi)\rho_c V^\dagger(\phi) + \cdots + V^{k-1}(\phi)\rho_c V^{\dagger k-1}(\phi)\right). \tag{26}$$

It is now possible to express the scaled s-th moment of quantum variable L, after the n-th step of the walk, in the suggestive form

$$\left\langle \left(\frac{L}{kn}\right)^s \right\rangle_n = \int_0^{2\pi} \frac{\rho(\phi,\phi)d\phi}{2\pi} (Tr_c[\sigma\varepsilon_\phi(\rho_c)])^s + O(n^{-1}). \tag{27}$$

Let us first elaborate on the first moment taken for $s = 1$ in last equation; to this end we introduce the $\phi-$average of the transformed density matrix $\varepsilon_\phi(\rho_c)$, with respect to the probability distribution function (pdf), ($\frac{\rho(\phi,\phi)}{2\pi}$, $0 < \phi \leq 2\pi$), that reads

$$\overline{\varepsilon}(\rho_c) = \int_0^{2\pi} \frac{\rho(\phi,\phi)d\phi}{2\pi} \varepsilon_\phi(\rho_c). \tag{28}$$

Then we obtain the first moment for $n >> 1$, in the form

$$\left\langle \left(\frac{L}{kn}\right) \right\rangle_\infty = Tr_c(\overline{\varepsilon}(\rho_c)\sigma) = \lim_{n\to\infty} \frac{1}{kn} Tr_w(\rho_w^{(n)} L). \tag{29}$$

This is interpreted as saying that (c.f. first eq. above) in the asymptotic regime of the walk, the expectation value of scaled variable L is proportional to the expectation value of observable σ, evaluated with the coin density matrix been transformed by the $\phi-$average of ε_ϕ. In the second equation above, it is emphasized that moment $\left\langle \left(\frac{L}{n}\right) \right\rangle_\infty$ is initially defined as expectation value of walker's space observable in the limit of large number of steps.

Next we continue our elaboration with the case for higher moments i.e $s > 1$. Referring to eq.(27), the integrand $(Tr_c[\sigma\varepsilon_\phi(\rho_c)])^s$, by means of the property of trace $Tr(A \otimes B) = TrA \cdot TrB$, or $TrA^{\otimes n} = (TrA)^n$, is expressed as $(Tr_c[\sigma\varepsilon_\phi(\rho_c)])^s = Tr_c[\sigma\varepsilon_\phi(\rho_c) \otimes \sigma\varepsilon_\phi(\rho_c) ... \otimes \sigma\varepsilon_\phi(\rho_c)]$. Further use of the property $A \otimes B \cdot C \otimes D = AC \otimes BD$, (dot sign emphasizes ordinary matrix product), and of notation $A^{\otimes n} = A \otimes A \otimes ... \otimes A$, for n-fold tensor product, yields that

$$(Tr_c[\sigma\varepsilon_\phi(\rho_c)])^s = Tr_c[\sigma^{\otimes s} \cdot \varepsilon_\phi(\rho_c) \otimes \varepsilon_\phi(\rho_c) \otimes ... \otimes \varepsilon_\phi(\rho_c)]. \tag{30}$$

We also need to introduce the $\phi-$average of the products of asymptotic density matrix $\varepsilon_\phi(\rho_c)$, appearing above i.e

$$\overline{\varepsilon^s}(\rho_c^{\otimes s}) = \int_0^{2\pi} \frac{\rho(\phi,\phi)d\phi}{2\pi} [\varepsilon_\phi(\rho_c) \otimes \varepsilon_\phi(\rho_c) \otimes ... \otimes \varepsilon_\phi(\rho_c)]. \tag{31}$$

Combining eqs. (30,31), we cast eq.(27) of the asymptotic s-th moment in following form

$$\left\langle \left(\frac{L}{kn}\right)^s \right\rangle_\infty = Tr_c[\sigma^{\otimes s}\overline{\varepsilon^s}(\rho_c^{\otimes s})] = \lim_{n\to\infty}\frac{1}{(kn)^s}Tr(\rho_w^{(n)}L^s) \tag{32}$$

Preceding equation (32) and its $s=1$ version in eq.(29), provide a framework for a quantum simulation of asymptotic statistics of quantum walk on a line. Such a framework identifies the walker system of a QRW with the system that is simulated by a second quantum system the simulator which in this case can be identified with the coin system of the QRW in question.

Indeed let us assume that we set up some appropriate Hamiltonian dynamics for a composite system comprised by a two-level atom identified with the coin system, and an ancillary system, so that after decoupling the two, by tracing out the ancilla system, the coins finds themselves in state $\overline{\varepsilon^s}(\rho_c)$. Then the quantum mean value of the observable $\sigma^{\otimes s}$, i.e. $\langle\sigma^{\otimes s}\rangle = Tr\sigma^{\otimes s}\overline{\varepsilon^s}(\rho_c)$, will be equal with the asymptotic s-th moment, of the walker system of the simulated QRW, by virtue of eq.(32). The problem of constructing appropriate

Hamiltonian dynamics has no unique solution, so next we provide a solution for the simplest nontrivial case of $k=2$. For this case eq.(26), becomes

$$\varepsilon_\phi(\rho_c) = \frac{1}{2}\left(\rho_c + V(\phi)\rho_c V^\dagger(\phi)\right). \tag{33}$$

To unitarize this transformation of coin density matrix we introduce a 2D auxiliary system, where $\rho_a = |+\rangle\langle+|$ is taken to be its density matrix. Then we find that

$$\varepsilon_\phi(\rho_c) = Tr_a W(\phi)(\rho_a\otimes\rho_c)W(\phi)^\dagger, \tag{34}$$

where the unitary matrix $W(\phi)$, is chosen to be

$$W(\phi) = \frac{1}{\sqrt{2}}(\mathbf{1}\otimes\mathbf{1} + |-\rangle\langle+|\otimes V(\phi) - |+\rangle\langle-|\otimes V(\phi)^\dagger) = \frac{1}{\sqrt{2}}\begin{pmatrix}\mathbf{1} & V(\phi)^\dagger\\ -V(\phi) & \mathbf{1}\end{pmatrix}. \tag{35}$$

Writing $W(\phi) = \exp H(\phi)$, the associated Hamiltonian matrix reads $H(\phi) = \frac{\pi}{4}[\sigma_+\otimes V(\phi)^\dagger - \sigma_-\otimes V(\phi)]$, so that if we choose the reshuffling matrix to be a $\frac{\pi}{4}$-rotation matrix, i.e. $V(\phi) = V_{cl}(\phi)U = e^{i\phi\sigma_3}U_{\frac{\pi}{4}} = e^{i\phi\sigma_3}e^{i\frac{\pi}{4}\sigma_2}$, then the Hamiltonian suggests a coupling of two spins and becomes

$$H(\phi) = \frac{\pi}{4}[\sigma_+\otimes e^{-i\frac{\pi}{4}\sigma_2}e^{-i\phi\sigma_3} - \sigma_-\otimes e^{i\phi\sigma_3}e^{i\frac{\pi}{4}\sigma_2}]. \tag{36}$$

Having constructed the Hamiltonian interaction that yields density matrix $\varepsilon_\phi(\rho_c)$, the $\phi-$averaged matrix $\overline{\varepsilon^s}(\rho_c)$, written in the form

$$\overline{\varepsilon^s}(\rho_c) = Tr_a \int_0^{2\pi} \frac{\rho(\phi,\phi)d\phi}{2\pi} \left[W(\phi)^{\otimes s} \left(\rho_a \otimes \rho_c\right)^{\otimes s} W(\phi)^{\otimes s\dagger} \right]. \tag{37}$$

requires the s-fold product unitary $W(\phi)^{\otimes s} = e^{\Delta H}$, with associated Hamiltonian the following multiple spin matrix $\Delta H = H \otimes \mathbf{1} \otimes ... \otimes \mathbf{1} + ... + \mathbf{1} \otimes ...\mathbf{1} \otimes H$. Explicitly it involves $2s$ two-level systems coupled in nearest neighbor form,

$$\begin{aligned} \Delta H \;=\; & \frac{\pi}{4}[\sigma_+ \otimes V(\phi)^\dagger - \sigma_- \otimes V(\phi)] \otimes \mathbf{1} \otimes ... \otimes \mathbf{1} + \frac{\pi}{4}\mathbf{1} \otimes [\sigma_+ \otimes V(\phi)^\dagger - \sigma_- \otimes V(\phi)] \otimes \mathbf{1} \otimes ... \otimes \mathbf{1} \\ & + \frac{\pi}{4}\mathbf{1} \otimes \mathbf{1} \otimes ... \otimes [\sigma_+ \otimes V(\phi)^\dagger - \sigma_- \otimes V(\phi)]. \end{aligned} \tag{38}$$

For example if initially $\rho_w = |0\rangle\langle 0|$, i.e. $\rho(\phi,\phi) = 1$, then the density matrix of eq.(37) is obtained by a uniform average of unitary similarity transformation generated by the Hamiltonian of last equation. Having constructed $\overline{\varepsilon^s}(\rho_c)$, by means of the evolution of simulator system, the moments of quantum walker's system are obtained by averaging measurements of observable $\sigma^{\otimes s}$, in accordance with eq.(32).

Classical Stochastic Simulation : An alternative way to implement physically the transformation outlined in eq.(28), is to consider the ensemble average of an appropriate stochastic unitary rotation acting on a two-level system. In more concrete terms, let us consider the angular random variable (rv) ϕ,distributed on circle by the pdf $\phi \sim (\frac{\rho(\phi,\phi)}{2\pi},\, 0 < \phi \leq 2\pi)$, and the independent discrete rv ν, uniformly distributed over the first k natural numbers i.e. $\nu \sim (\{0,1,...,k-1\})$. Then we form a transformation of the coin density matrix as follows $\rho_c \to V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu}$. This is a random similarity transformation of the density matrix with the random unitary matrix $V(\phi)^\nu$; its randomness is both due to angle ϕ and due to exponent ν. Taking the statistical average of this transformation over its two rv's with respect to their corresponding pdf's to be denoted by $\left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_{\phi,\nu}$, we write that

$$\left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_{\phi,\nu} = \frac{1}{k} \int_0^{2\pi} \frac{\rho(x,x)dx}{2\pi} \left(\sum_{m=0}^{k-1} V(x)^m \rho_c V(x)^{\dagger m} \right) \equiv \overline{\varepsilon}(\rho_c). \tag{39}$$

This is identical with eq.(28); note also that due to the statistical independence of ϕ and ν variables, the double statistical mean of rotations is obtained by evaluating successively the mean for each variable i.e. $\overline{\varepsilon}(\rho_c) = \left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_{\phi,\nu} = \left\langle \left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_\phi \right\rangle_\nu = \left\langle \left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_\nu \right\rangle_\phi$.

This same implementation idea is further generalized to get the analogue of eq.(37). For that s identical two-level systems are needed together with s identical and statistically independent discrete random variables, uniformly distributed over the first k natural numbers i.e. $\nu_i \sim (\{0, 1, ..., k-1\})$, $i = 1, 2, ..., s$, as well as an independent circular rv $\phi \sim (\frac{\rho(\phi,\phi)}{2\pi}$, $0 < \phi \leq 2\pi)$. First we form the statistical average over the s independent discrete variables

$$\varepsilon_\phi(\rho_c) \otimes ... \otimes \varepsilon_\phi(\rho_c) = \left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_\nu \otimes ... \otimes \left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_\nu . \tag{40}$$

Then we treat the resulting s-fold tensor product of density matrices $\varepsilon_\phi(\rho_c)$, as ϕ correlated matrix-valued random variables, and consider their statistical average

$$\left\langle \varepsilon_\phi(\rho_c) \otimes ... \otimes \varepsilon_\phi(\rho_c) \right\rangle_\phi = \int_0^{2\pi} \frac{\rho(\phi,\phi)d\phi}{2\pi} \left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_\nu \otimes ... \otimes \left\langle V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu} \right\rangle_\nu . \tag{41}$$

The doubly averaged density matrix is identical to $\overline{\varepsilon^s}(\rho_c)$, i.e. $\overline{\varepsilon^s}(\rho_c) = \left\langle \varepsilon_\phi(\rho_c) \otimes ... \otimes \varepsilon_\phi(\rho_c) \right\rangle_\phi$.

We note finally that the range k of discrete rv ν is determined by the kind of V^k model of QRW the statistical moments of which we simulate, and that similarly the number s of two-level atoms involved in simulation is determined by the order of quantum moment of walker's system we intend to simulate. Two-level atoms, and the ϕ, ν, classical stochastic variables are quantum and classical resources required for this *on the average* stochastic simulation of QRW. Note also that, the main difference between quantum and stochastic simulations is in the way the CPTP maps of coin systems are derived: in the stochastic case many runs of random rotations are required so that a classical ensemble average is formed, while in quantal case the prescribed total unitary evolution is generated in one run and then an coin unconditional measurement provides the final density matrix (c.f. 34-37).

As to the experimental realization of the proposed stochastic implementation we note that the transformation $\rho_c \to V(\phi)^\nu \rho_c V(\phi)^{\dagger\nu}$, requires a random rotation $V(\phi)^\nu = (V_{cl}(\phi)U)^\nu = (e^{i\phi\sigma_3} e^{i\frac{\pi}{4}\sigma_2})^\nu$. For the case of $k = 2$, i.e. $\nu = 0, 1$, we need to flip randomly between the two rotations ($\mathbf{1}$,$e^{i\phi\sigma_3} e^{i\frac{\pi}{4}\sigma_2}$), of the coin system. Stochastic unitary rotations of a two-level atom can experimentally be achieved by randomly pulsating laser fields with appropriate fluctuating phases and intensities [34].

As corroboration of our theoretical results about quantum simulation, we next provide numerical evaluation of the asymptotic probability density function of the walker. This is

done for the example of $U-$quantization (c.f. eq.(24) for the models with $k = 2, 3$), and the example of $\varepsilon-$quantization (c.f. eq.(19)). If $Y = h(\phi)$, then the cumulative probability function in the interval $[y_1, y_2]$ becomes

$$P(y_1 \leq Y \leq y_2) = \frac{1}{2\pi} \int\limits_{y_1 \leq h(\phi) \leq y_2} \rho(\phi, \phi) d\phi. \tag{42}$$

In the application we choose $\rho(\phi, \phi) = 1$,corresponding to $\rho_w = |0\rangle\langle 0|$. In the numerical simulation to determine the values of the probability density function over some small interval $I = [a, b]$, we count the number of times the random variable ϕ, is such that $y_1 \leq h(\phi) \leq y_2$, and compute the fraction of the number of successful counts by the overall number of counts. The results displayed in fig. 1a, for the model V^2, quantized by the U-rule, show the well known by now double-horn distribution (c.f. previous works cited in the introductory chapter). As to the results of fig.1b and fig.2, they are new, and provide information about the asymptotic behavior of the $k = 3$ model quantized by $U-$rule, and of the model $k = 2$, quantized according to $\varepsilon-$quantization rule. The results show some similarity in the form of the distributions, but also important differences in the displacements and the cutoffs of their supports. These should be detectable features in realistic simulations of a walk with quantum systems. Finally, these results should be compared and constrasted with those of [15]. In that work the delayed tracing scheme with time step evolution maps ε_V, ε_{V^2}, ε_{V^3}, ..., [22], was used for QRW on line, in which coin decoherence has been introduced, and modifies the quantum walk along the lines of $\varepsilon-$quantization rule. These results show destruction of quantum features of the walk for increasing strength of decoherence. On the contrary results indicated in fig. 2, show that for the analogous $\varepsilon-$quantized ε_{V^2} model with $\varepsilon^n_{V^2}$, $n = 1, 2, ...$, time step evolution maps, the quantum features are retained in the long time regime, albeit in a modified form.

V. CONCLUSIONS

Quantization rules provide a broad and systematic framework for quantizing classical random walks, taking into account phenomena such as losses, decoherence, noise or coherent dynamics occurring in the coin systems. Optical processes that may cause or on purpose induce similar phenomena in coins may therefore constitute physical probes for the study of novel features in quantum walks. The prospects of such quantum optical walks are further

enhanced by the possibility of using the coin systems not only as a trigger of the walk, but also as a quantum simulator of its dynamics and statistics, especially of its long terms characteristics [35]. In this framework phenomena related to quantum-classical transitions in walker's evolution, and to quantum coin+walker entanglement, especially in the asymptotic regime of a walk, find new theoretical and experimental possibilities for a in-depth investigation. To some of these topics we aim to return elsewhere.

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[35] More generally, quantum coin systems interacting with quantum walker systems to form a QRW, do not necesserily have to be two different systems brought in physical contact, but may constitute two interacting degrees of freedom of a single quantum system, see e.g. A. J. Bracken, D. Ellinas and I. Smyrnakis, ArXiv:quant-ph/0605195, in where the spin (coin) and positional (walker) degree of freedom of a Dirac relativistic electron, implement naturally the evolution of a QRW and reproduce its asympotic behaviour.

Figure captions

Figure 1a,1b

Asymptotic probability density function, for walker's scaled position variable. It refers to the V^2 model in fig. 1a (the V^3 model in fig. 1b), quantized by the U-rule, with reshuffling matrix the $\frac{\pi}{4}$ rotation matrix, and initial coin chosen in excited state.

Figure 2

Asymptotic probability density function, for walker's scaled position variable. It refers to the V^2 model, quantized by the ε-rule, with initial coin chosen in excited state.

Fig. 1a U−quantized walk : simulation of asymptotic density function of the walker, k=2

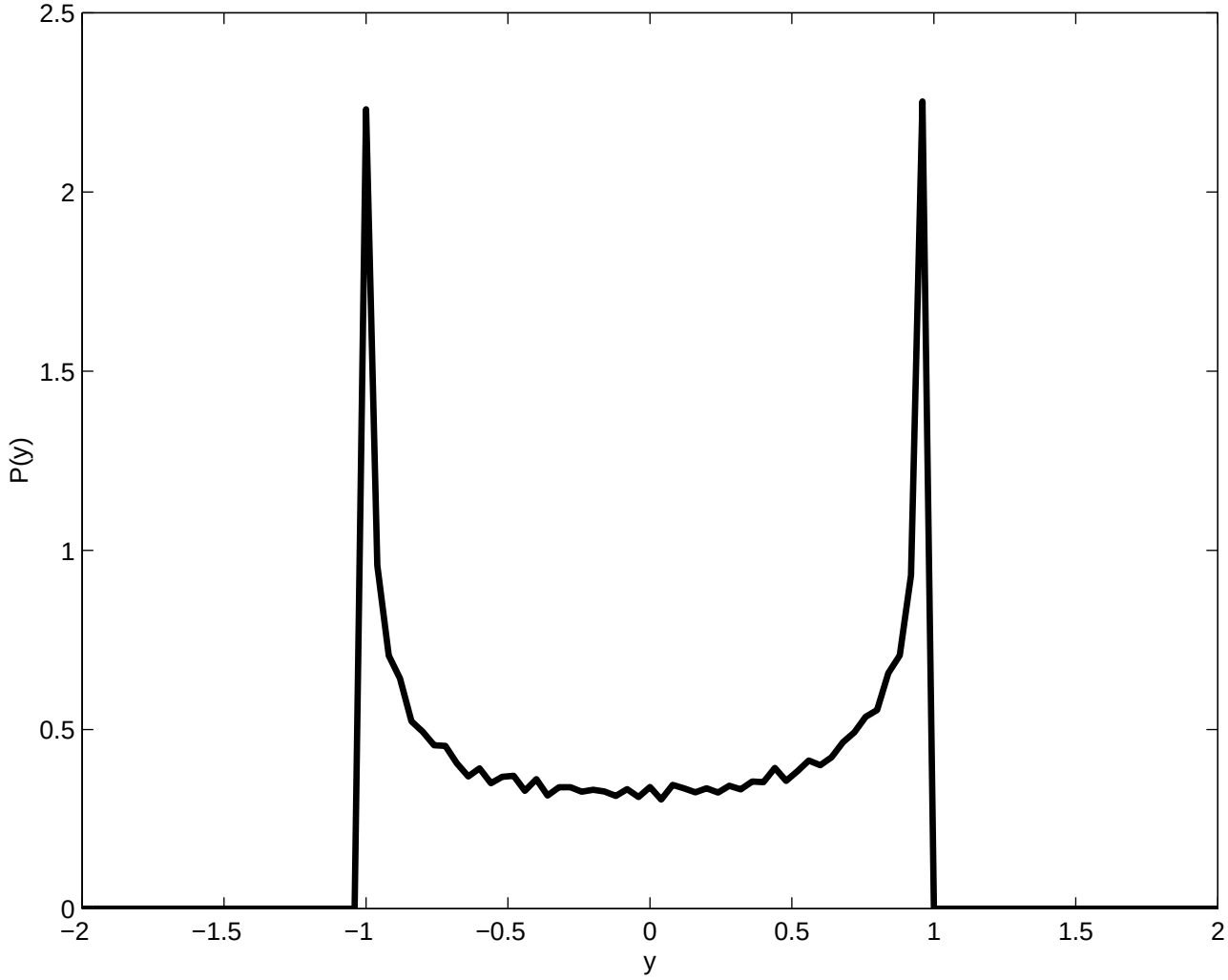

Fig. 1b U−quantized walk : simulation of asymptotic density function of the walker, k=3

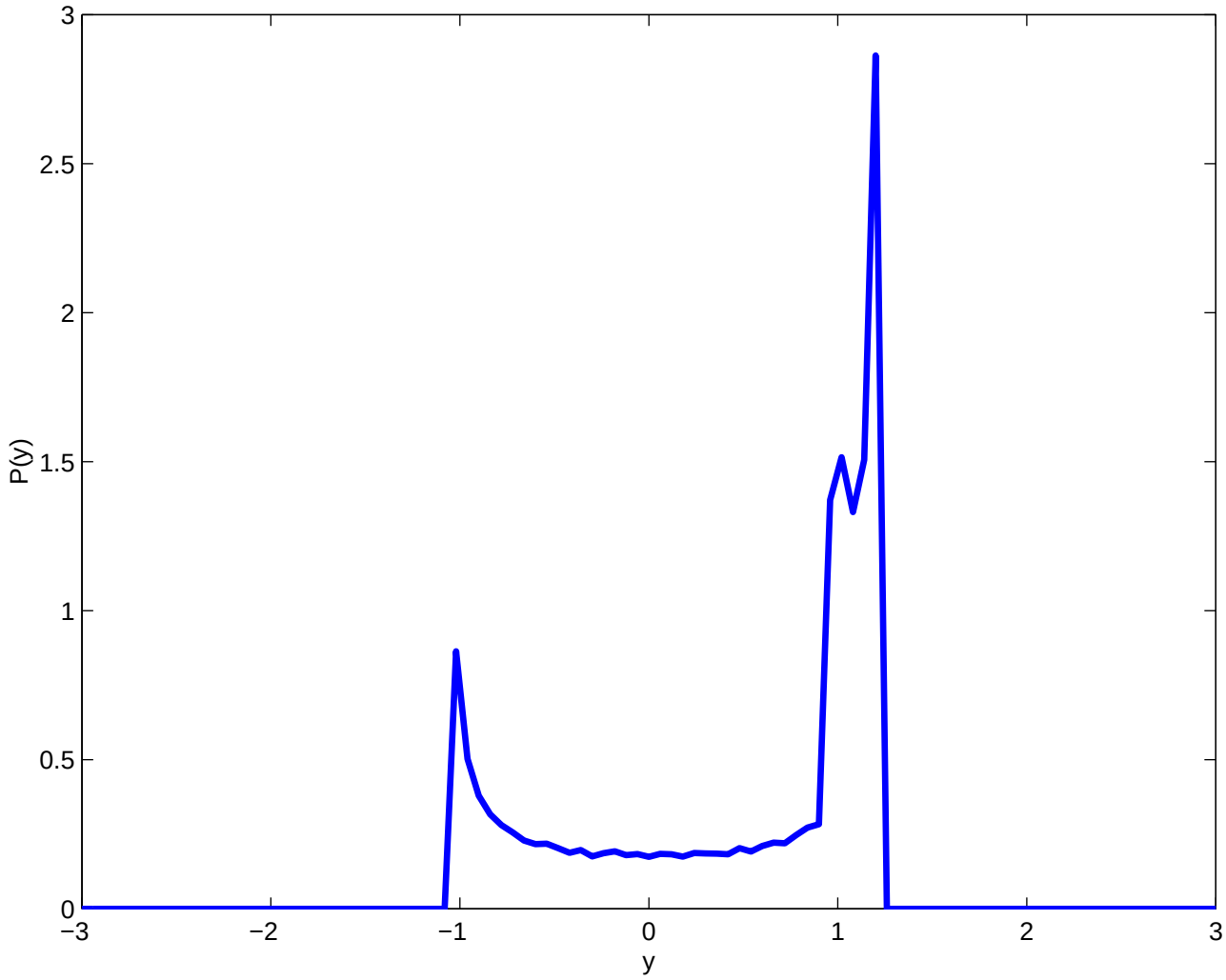

Fig.2 Epsilon−quantized walk : simulation of asymptotic probability density function of the walker